Learning Gradient Fields for Molecular Conformation Generation

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Abstract

We study a fundamental problem in computational chemistry known as molecular conformation generation, trying to predict stable 3D structures from 2D molecular graphs. Existing machine learning approaches usually first predict distances between atoms and then generate a 3D structure satisfying the distances, where noise in predicted distances may induce extra errors during 3D coordinate generation. Inspired by the traditional force field methods for molecular dynamics simulation, in this paper, we propose a novel approach called ConfGF by directly estimating the gradient fields of the log density of atomic coordinates. The estimated gradient fields allow directly generating stable conformations via Langevin dynamics. However, the problem is very challenging as the gradient fields are roto-translation equivariant. We notice that estimating the gradient fields of atomic coordinates can be translated to estimating the gradient fields of interatomic distances, and hence develop a novel algorithm based on recent score-based generative models to effectively estimate these gradients. Experimental results across multiple tasks show that ConfGF outperforms previous state-of-the-art baselines by a significant margin.